

χ^2 -confidence sets in high-dimensional regression

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Abstract We study a high-dimensional regression model. Aim is to construct a confidence set for a given group of regression coefficients, treating all other regression coefficients as nuisance parameters. We apply a one-step procedure with the square-root Lasso as initial estimator and a multivariate square-root Lasso for constructing a surrogate Fisher information matrix. The multivariate square-root Lasso is based on nuclear norm loss with ℓ_1 -penalty. We show that this procedure leads to an asymptotically χ^2 -distributed pivot, with a remainder term depending only on the ℓ_1 -error of the initial estimator. We show that under ℓ_1 -sparsity conditions on the regression coefficients β^0 the square-root Lasso produces to a consistent estimator of the noise variance and we establish sharp oracle inequalities which show that the remainder term is small under further sparsity conditions on β^0 and compatibility conditions on the design.

1 Introduction

Let X be a given $n \times p$ input matrix and Y be a random n -vector of responses. We consider the high-dimensional situation where the number of variables p exceeds the number of observations n . The expectation of Y (assumed to exist) is denoted by $f^0 := \mathbb{E}Y$. We assume that X has rank n ($n < p$) and let β^0 be any solution of the equation $X\beta^0 = f^0$. Our aim is to construct a confidence interval for a pre-specified group of coefficients $\beta_J^0 := \{\beta_j^0 : j \in J\}$ where $J \subset \{1, \dots, p\}$ is a subset of the indices. In other words, the $|J|$ -dimensional vector β_J^0 is the parameter of interest and all the other coefficients $\beta_{-J}^0 := \{\beta_j^0 : j \notin J\}$ are nuisance parameters.

For one-dimensional parameters of interest ($|J| = 1$) the approach in this paper is closely related to earlier work. The method is introduced in Zhang and Zhang [2014]. Further references are Javanmard and Montanari [2013] and van de Geer et al. [2014]. Related approaches can be found in Belloni et al. [2013a], Belloni et al. [2013b] and Belloni et al. [2014].

For confidence sets for groups of variables ($|J| > 1$) one usually would like to take the dependence between estimators of single parameters into account. An important paper that carefully does this for confidence sets in ℓ_2 is Mitra and Zhang [2014]. Our approach is

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related but differs in an important way. As in Mitra and Zhang [2014] we propose a de-sparsified estimator which is (potentially) asymptotically linear. However, Mitra and Zhang [2014] focus at a remainder term which is small also for large groups. Our goal is rather to present a construction which has a small remainder term after studentizing and which does not rely on strong conditions on the design X . In particular we do not assume any sparsity conditions on the design.

The construction involves the square-root Lasso $\hat{\beta}$ which is introduced by Belloni et al. [2011]. See Section 2 for the definition of the estimator $\hat{\beta}$. We present a multivariate extension of the square-root Lasso which takes the nuclear norm of the multivariate residuals as loss function. Then we define in Section 3.1 a de-sparsified estimator \hat{b}_J of β_J^0 which has the form of a one-step estimator with $\hat{\beta}_J$ as initial estimator and with multivariate square-root Lasso invoked to obtain a surrogate Fisher information matrix. We show that when $Y \sim \mathcal{N}_n(f^0, \sigma_0^2 I)$ (with both f^0 and σ_0^2 unknown), a studentized version of $\hat{b}_J - \beta_J^0$ has asymptotically a $|J|$ -dimensional standard normal distribution.

More precisely we will show in Theorem 1 that for a given $|J| \times |J|$ matrix $M = M_\lambda$ depending only on X and on a tuning parameter λ , one has $M_\lambda(\hat{b}_J - \beta_J^0)/\sigma_0 = \mathcal{N}_{|J|}(0, I) + \text{rem}$ where the remainder term “rem” can be bounded by $\|\text{rem}\|_\infty \leq \sqrt{n}\lambda \|\hat{\beta}_{-J} - \beta_{-J}^0\|_1/\sigma_0$. The choice of the tuning parameter λ is “free” (and not depending on σ_0), it can for example be taken of order $\sqrt{\log p/n}$. The unknown parameter σ_0^2 can be estimated by the normalized residual sum of squares $\hat{\sigma}^2 := \|Y - X\hat{\beta}\|_2^2/n$ of the square-root Lasso $\hat{\beta}$. We show in Lemma 3 that under sparsity conditions on β^0 one has $\hat{\sigma}^2/\sigma_0^2 = 1 + o_P(1)$ and then in Theorem 2 an oracle inequality for the square-root Lasso under further sparsity conditions on β^0 and compatibility conditions on the design. The oracle result allows one to “verify” when $\sqrt{n}\lambda \|\hat{\beta}_{-J} - \beta_{-J}^0\|_1/\sigma_0 = o_P(1)$ so that the remainder term rem is negligible. An illustration assuming weak sparsity conditions is given in Section 5. As a consequence

$$\|M_\lambda(\hat{b}_J - \beta_J^0)\|_2^2/\hat{\sigma}^2 = \chi_{|J|}^2(1 + o_P(1)),$$

where $\chi_{|J|}^2$ is a random variable having a χ^2 -distribution with $|J|$ degrees of freedom. For $|J|$ fixed one can thus construct asymptotic confidence sets for β_J^0 (we will also consider the case $|J| \rightarrow \infty$ in Section 8). We however do not control the size of these sets. Larger values for λ makes the confidence sets smaller but will also give a larger remainder term.

In Section 6 we extend the theory to structured sparsity norms other than ℓ_1 , for example the norm used for the (square-root) group Lasso, where the demand for ℓ_2 -confidence sets for groups comes up quite naturally. Section 8 contains a discussion. The proofs are in Section 9.

1.1 Notation

The mean vector of Y is denoted by f^0 and the noise is $\varepsilon := Y - f^0$. For a vector $v \in \mathbb{R}^n$ we write (with a slight abuse of notation) $\|v\|_n^2 := v^T v/n$. We let $\sigma_0^2 := \mathbb{E}\|\varepsilon\|_n^2$ (assumed to exist).

For a vector $\beta \in \mathbb{R}^p$ we set $S_\beta := \{j : \beta_j \neq 0\}$. For a subset $J \subset \{1, \dots, p\}$ and a vector $\beta \in \mathbb{R}^p$ we use the same notation β_J for the $|J|$ -dimensional vector $\{\beta_j : j \in J\}$ and the p -dimensional vector $\{\beta_{j,J} := \beta_j 1\{j \in J\} : j = 1, \dots, p\}$. The last version allows us to write $\beta = \beta_J + \beta_{-J}$ with $\beta_{-J} = \beta_{J^c}$, J^c being the complement of the set J . The j -th column of X is denoted by X_j ($j = 1, \dots, p$). We let $X_J := \{X_j : j \in J\}$ and $X_{-J} := \{X_j : j \notin J\}$.

For a matrix A we let $\|A\|_{\text{nuclear}} := \text{trace}((A^T A)^{1/2})$ be its nuclear norm. The ℓ_1 -norm of the matrix A is defined as $\|A\|_1 := \sum_k \sum_j |a_{k,j}|$. Its ℓ_∞ -norm is $\|A\|_\infty := \max_k \max_j |a_{k,j}|$.

2 The square-root Lasso and its multivariate version

2.1 The square-root Lasso

The square-root Lasso (Belloni et al. [2011]) $\hat{\beta}$ is

$$\hat{\beta} := \arg \min_{\beta \in \mathbb{R}^p} \left\{ \|Y - X\beta\|_n + \lambda_0 \|\beta\|_1 \right\}. \quad (1)$$

The parameter $\lambda_0 > 0$ is a tuning parameter. Thus $\hat{\beta}$ depends on λ_0 but we do not express this in our notation.

The square-root Lasso can be seen as a method that estimates β^0 and the noise variance σ_0^2 simultaneously. Defining the residuals $\hat{\varepsilon} := Y - X\hat{\beta}$ and letting $\hat{\sigma}^2 := \|\hat{\varepsilon}\|_n^2$ one clearly has

$$(\hat{\beta}, \hat{\sigma}^2) = \arg \min_{\beta \in \mathbb{R}^p, \sigma^2 > 0} \left\{ \frac{\|Y - X\beta\|_n^2}{\sigma} + \sigma + 2\lambda_0 \|\beta\|_1 \right\} \quad (2)$$

provided the minimum is attained at a positive value of σ^2 .

We note in passing that the square-root Lasso is *not* a quasi-likelihood estimator as the function $\exp[-z^2/\sigma - \sigma]$, $z \in \mathbb{R}$, is not a density with respect to a dominating measure not depending on $\sigma^2 > 0$. The square-root Lasso is moreover not to be confused with the scaled Lasso. The latter is a quasi-likelihood estimator. It is studied in e.g. Sun and Zhang [2012].

We show in Section 4.1 (Lemmas 2 and 3) that for the case where $\varepsilon \sim \mathcal{N}_n(0, \sigma_0^2 I)$ for example one has $\hat{\sigma} \rightarrow \sigma_0$ under ℓ_1 -sparsity conditions on β^0 . In Section 4.2 we establish oracle results for $\hat{\beta}$ under further sparsity conditions on β^0 and compatibility conditions on X (see Definition 2 for the latter). These results hold for a “universal” choice of λ_0 provided an ℓ_1 -sparsity condition on β^0 is met.

In the proof of our main result in Theorem 1, the so-called *Karush-Kuhn-Tucker conditions*, or KKT-conditions, play a major role. Let us briefly discuss these here. The KKT-conditions for the square-root Lasso say that

$$\frac{X^T(Y - X\hat{\beta})/n}{\hat{\sigma}} = \lambda_0 \hat{z} \quad (3)$$

where \hat{z} is a p -dimensional vector with $\|\hat{z}\|_\infty \leq 1$ and with $\hat{z}_j = \text{sign}(\hat{\beta}_j)$ if $\hat{\beta}_j \neq 0$. This follows from sub-differential calculus which defines the sub-differential of the absolute value function $x \mapsto |x|$ as

$$\{\text{sign}(x)\}\{x \neq 0\} + [-1, 1]\{x = 0\}.$$

Indeed, for a fixed $\sigma > 0$ the sub-differential with respect to β of the expression in curly brackets given in (2) is equal to

$$-\frac{2X^T(Y - X\beta)/n}{\sigma} + 2\lambda_0 z(\beta)$$

with, for $j = 1, \dots, p$, $z_j(\beta)$ the sub-differential of $\beta_j \mapsto |\beta_j|$. Setting this to zero at $(\hat{\beta}, \hat{\sigma})$ gives the above KKT-conditions (3).

2.2 The multivariate square-root Lasso

In our construction of confidence sets we will consider the regression of X_J on X_{-J} invoking a multivariate version of the square-root Lasso. To explain the latter, we use here a standard notation with X being the input and Y being the response. We will then replace X by X_{-J} and Y by X_J in Section 3.1.

The matrix X is as before an $n \times p$ input matrix and the response Y is now an $n \times q$ matrix for some $q \geq 1$. We define the multivariate square-root Lasso

$$\hat{B} := \arg \min_B \left\{ \|Y - XB\|_{\text{nuclear}} / \sqrt{n} + \lambda_0 \|B\|_1 \right\} \quad (4)$$

with $\lambda_0 > 0$ again a tuning parameter. The minimization is over all $p \times q$ matrices B . We consider $\hat{\Sigma} := (Y - X\hat{B})^T (Y - X\hat{B}) / n$ as estimator of the noise co-variance matrix.

The KKT-conditions for the multivariate square-root Lasso will be a major ingredient of the proof of the main result in Theorem 1. We present these KKT-conditions in the following lemma in equation (5).

Lemma 1. *We have*

$$\begin{aligned} (\hat{B}, \hat{\Sigma}) = \arg \min_{B, \Sigma > 0} & \left\{ \text{trace} \left((Y - XB)^T (Y - XB) \Sigma^{-1/2} \right) / n \right. \\ & \left. + \text{trace}(\Sigma^{1/2}) + 2\lambda_0 \|B\|_1 \right\} \end{aligned}$$

where the minimization is over all symmetric positive definite matrix Σ (this being denoted by $\Sigma > 0$) and where it is assumed that the minimum is indeed attained at some $\Sigma > 0$. The multivariate Lasso satisfies the KKT-conditions

$$X^T (Y - X\hat{B}) \hat{\Sigma}^{-1/2} / n = \lambda_0 \hat{Z}, \quad (5)$$

where \hat{Z} is a $p \times q$ matrix with $\|\hat{Z}\|_\infty \leq 1$ and with $\hat{Z}_{k,j} = \text{sign}(\hat{B}_{k,j})$ if $\hat{B}_{k,j} \neq 0$ ($k = 1, \dots, p$, $j = 1, \dots, q$).

3 Confidence sets for β_J^0

3.1 The construction

Let $J \subset \{1, \dots, p\}$. We are interested in building a confidence set for $\beta_J^0 := \{\beta_j^0 : j \in J\}$. To this end, we compute the multivariate ($|J|$ -dimensional) square root Lasso

$$\hat{\Gamma}_J := \arg \min_{\Gamma_J} \left\{ \|X_J - X_{-J}\Gamma_J\|_{\text{nuclear}} / \sqrt{n} + \lambda \|\Gamma_J\|_1 \right\} \quad (6)$$

where $\lambda > 0$ is a tuning parameter. The minimization is over all $(p - |J|) \times |J|$ matrices Γ_J . We let

$$\tilde{T}_J := (X_J - X_{-J}\hat{\Gamma}_J)^T X_J / n \quad (7)$$

and

$$\hat{T}_J := (X_J - X_{-J}\hat{\Gamma}_J)^T (X_J - X_{-J}\hat{\Gamma}_J) / n, \quad (8)$$

We assume throughout that the “hat” matrix \hat{T}_J is non-singular. The “tilde” matrix \tilde{T}_J only needs to be non-singular in order that the de-sparsified estimator \hat{b}_J given below in Definition 1 is well-defined. However, for the normalized version we need not assume non-singularity of \tilde{T}_J .

The KKT-conditions (5) appear in the form

$$X_{-J}^T (X_J - X_{-J}\hat{\Gamma}_J) \hat{T}_J^{-1/2} / n = \lambda \hat{Z}_J, \quad (9)$$

where \hat{Z}_J is a $(p - |J|) \times |J|$ matrix with $(\hat{Z}_J)_{k,j} = \text{sign}(\hat{\Gamma}_J)_{k,j}$ if $(\hat{\Gamma}_J)_{k,j} \neq 0$ and $\|\hat{Z}_J\|_\infty \leq 1$.

We define the normalization matrix

$$M := M_\lambda := \sqrt{n} \hat{T}_J^{-1/2} \tilde{T}_J. \quad (10)$$

Definition 1. The de-sparsified estimator of β_J^0 is

$$\hat{b}_J := \hat{\beta}_J + \tilde{T}_J^{-1} (X_J - X_{-J}\hat{\Gamma}_J)^T (Y - X\hat{\beta}) / n,$$

with $\hat{\beta}$ the square-root Lasso given in (1), $\hat{\Gamma}_J$ the multivariate square-root Lasso given in (6) and the matrix \tilde{T}_J given in (7). The normalized de-sparsified estimator is $M\hat{b}_J$ with M the normalization matrix given in (10).

3.2 The main result

Our main result is rather simple. It shows that using the multivariate square-root Lasso for de-sparsifying, and then normalizing, results in a well-scaled “asymptotic pivot” (up to the estimation of σ_0 which we will do in the next section). Theorem 1 actually does not require $\hat{\beta}$ to be the square-root Lasso but for definiteness we have made this specific choice throughout the paper (except for Section 6).

Theorem 1. Consider the model $Y \sim \mathcal{N}_n(f^0, \sigma_0^2)$ where $f^0 = X\beta^0$. Let \hat{b}_J be the de-sparsified estimator given in Definition 1 and let $M\hat{b}_J$ be its normalized version. Then

$$M(\hat{b}_J - \beta_J^0) / \sigma_0 = \mathcal{N}_{|J|}(0, I) + \text{rem}$$

where $\|\text{rem}\|_\infty \leq \sqrt{n}\lambda \|\hat{\beta}_{-J} - \beta_{-J}^0\|_1 / \sigma_0$.

To make Theorem 1 work we need to bound $\|\hat{\beta} - \beta^0\|_1 / \hat{\sigma}$ where $\hat{\sigma}$ is an estimator of σ_0 . This is done in Theorem 2 with $\hat{\sigma}$ the estimator $\|\hat{\epsilon}\|_n$ from the square-root Lasso. A special case is presented in Lemma 5 which imposes weak sparsity conditions for β^0 . Bounds for $\sigma_0 / \hat{\sigma}$ are also given.

Theorem 1 is about the case where the noise ϵ is i.i.d. normally distributed. This can be generalized as from the proof we see that the “main” term is linear in ϵ . For independent errors with common variance σ_0^2 say, one needs to assume the Lindeberg condition for establishing asymptotic normality.

4 Theory for the square root Lasso

Let $f^0 := \mathbb{E}Y$, β^0 be a solution of $X\beta^0 = f^0$ and define $\varepsilon := Y - f^0$. Recall the square-root Lasso $\hat{\beta}$ given in (1). It depends on the tuning parameter $\lambda_0 > 0$. In this section we develop theoretical bounds, which are closely related to results in Sun and Zhang [2013] (who by the way use the term scaled Lasso instead of square-root Lasso in that paper). There are two differences. Firstly, our lower bound for the residual sum of squares of the square-root Lasso requires, for the case where no conditions are imposed on the compatibility constants, a smaller value for the tuning parameter (see Lemma 3). These compatibility constants, given in Definition 2, are required only later for the oracle results. Secondly, we establish an oracle inequality that is sharp (see Theorem 2 in Section 4.2 where we present more details).

Write $\hat{\varepsilon} := Y - X\hat{\beta}$ and $\hat{\sigma}^2 := \|\hat{\varepsilon}\|_n^2$. We consider bounds in terms of $\|\varepsilon\|_n^2$, the “empirical” variance of the unobservable noise. This is a random quantity but under obvious conditions it converges to its expectation σ_0^2 . Another random quantity that appears in our bounds is $\varepsilon/\|\varepsilon\|_n$, which is a random point on the n -dimensional unit sphere. We write

$$\hat{R} := \frac{\|X^T \varepsilon\|_\infty}{n\|\varepsilon\|_n}.$$

When all X_j are normalized such that $\|X_j\|_n = 1$, the quantity \hat{R} is the maximal “empirical” correlation between noise and input variables. Under distributional assumptions \hat{R} can be bounded with large probability by some constant R . For completeness we work out the case of i.i.d. normally distributed errors.

Lemma 2. *Let $\varepsilon \sim \mathcal{N}_n(0, \sigma_0^2 I)$. Suppose the normalized case where $\|X_j\|_n = 1$ for all $j = 1, \dots, p$. Let α_0 , $\underline{\alpha}$ and $\bar{\alpha}$ be given positive error levels such that $\alpha_0 + \underline{\alpha} + \bar{\alpha} < 1$ and $\log(1/\underline{\alpha}) < n/4$. Define*

$$\begin{aligned} \underline{\sigma}^2 &:= \sigma_0^2 \left(1 - 2\sqrt{\frac{\log(1/\underline{\alpha})}{n}} \right), \\ \bar{\sigma}^2 &:= \sigma_0^2 \left(1 + 2\sqrt{\frac{\log(1/\bar{\alpha})}{n}} + \frac{2\log(1/\bar{\alpha})}{n} \right) \end{aligned}$$

and

$$R := \sqrt{\frac{\log(2p/\alpha_0)}{n - 2\sqrt{n\log(1/\underline{\alpha})}}}.$$

We have

$$\mathbf{P}(\|\varepsilon\|_n \leq \underline{\sigma}) \leq \underline{\alpha}, \quad \mathbf{P}(\|\varepsilon\|_n \geq \bar{\sigma}) \leq \bar{\alpha}$$

and

$$\mathbf{P}(\hat{R} \geq R \cup \|\varepsilon\|_n \leq \underline{\sigma}) \leq \alpha_0 + \underline{\alpha}.$$

4.1 Preliminary lower and upper bounds for $\hat{\sigma}^2$

We now show that the estimator of the variance $\hat{\sigma}^2 = \|\hat{\varepsilon}\|_n^2$, obtained by applying the square-root Lasso, converges to the noise variance σ_0^2 . The result holds without conditions on compatibility constants (given in Definition 2). We do however need the ℓ_1 -sparsity condition (11) on β_0 . This condition will be discussed below in an asymptotic setup.

Lemma 3. Suppose that for some $0 < \eta < 1$, some $R > 0$ and some $\underline{\sigma} > 0$, we have

$$\lambda_0(1 - \eta) \geq R$$

and

$$\lambda_0 \|\beta^0\|_1 / \underline{\sigma} \leq 2 \left(\sqrt{1 + (\eta/2)^2} - 1 \right). \quad (11)$$

Then on the set where $\hat{R} \leq R$ and $\|\varepsilon\|_n \geq \underline{\sigma}$ we have $\left| \|\hat{\varepsilon}\|_n / \|\varepsilon\|_n - 1 \right| \leq \eta$.

We remark here that the result of Lemma 3 is also useful when using a square-root Lasso for constructing an asymptotic confidence interval for a single parameter, say β_j^0 . Assuming random design it can be applied to show that without imposing compatibility conditions the residual variance of the square root Lasso for the regression of X_j on all other variables X_{-j} does not degenerate.

Asymptotics Suppose $\varepsilon_1, \dots, \varepsilon_n$ are i.i.d. with finite variance σ_0^2 . Then clearly $\|\varepsilon\|_n / \sigma_0 \rightarrow 1$ in probability. The normalization in (11) by $\underline{\sigma}$ - which can be taken more or less equal to σ_0 - makes sense if we think of the standardized model

$$\tilde{Y} = X\tilde{\beta}^0 + \tilde{\varepsilon},$$

with $\tilde{Y} = Y/\sigma_0$, $\tilde{\beta}^0 = \beta^0/\sigma_0$ and $\tilde{\varepsilon} = \varepsilon/\sigma_0$. The condition (11) is a condition on the normalized $\tilde{\beta}^0$. The rate of growth assumed there is quite common. First of all, it is clear that if $\|\beta^0\|_1$ is very large then the estimator is not very good because of the penalty on large values of $\|\cdot\|_1$. The condition (11) is moreover closely related to standard assumptions in compressed sensing. To explain this we first note that

$$\|\beta^0\|_1 / \sigma_0 \leq \sqrt{s_0} \|\beta^0\|_2 / \sigma_0$$

when s_0 is the number of non-zero entries of β^0 (observe that s_0 is a scale free property of β^0). The term $\|\beta^0\|_2 / \sigma_0$ can be seen as a signal-to-noise ratio. Let us assume this signal-to-noise ratio stays bounded. If λ_0 corresponds to the standard choice $\lambda_0 \asymp \sqrt{\log p/n}$ the assumption (11) holds with $\eta = o(1)$ as soon as we assume the standard assumption $s_0 = o(n/\log p)$.

4.2 An oracle inequality for the square-root Lasso

Our next result is an oracle inequality for the square-root Lasso. It is as the corresponding result for the Lasso as established in Bickel et al. [2009]. The oracle inequality of Theorem 2 is sharp in the sense that there is a constant 1 in front of the approximation error $\|X(\beta - \beta^0)\|_n^2$ in (12). This sharpness is obtained along the lines of arguments from Koltchinskii et al. [2011], who prove sharp oracle inequalities for the Lasso and for matrix problems. We further have extended the situation in order to establish an oracle inequality for the ℓ_1 -estimation error $\|\hat{\beta} - \beta^0\|_1$ where we use arguments from van de Geer [2014] for the Lasso. For the square-root Lasso, the paper Sun and Zhang [2013] also has oracle inequalities, but these are not sharp.

Compatibility constants are introduced in van de Geer [2007]. They play a role in the identifiability of β^0 .

Definition 2. Let $L > 0$ and $S \subset \{1, \dots, p\}$. The compatibility constant is

$$\hat{\phi}^2(L, S) = \min \left\{ |S| \|X\beta\|_n^2 : \|\beta_S\|_1 = 1, \|\beta_{-S}\|_1 \leq L \right\}.$$

We recall the notation $S_\beta = \{j : \beta_j \neq 0\}$ appearing in (12).

Theorem 2. *Let λ_0 satisfy for some $R > 0$*

$$\lambda_0(1 - \eta) > R$$

and assume the ℓ_1 -sparsity (11) for some $0 < \eta < 1$ and $\underline{\sigma} > 0$, i.e.

$$\lambda_0 \|\beta^0\|_1 / \underline{\sigma} \leq 2 \left(\sqrt{1 + (\eta/2)^2} - 1 \right).$$

Let $0 \leq \delta < 1$ be arbitrary and define

$$\underline{\lambda} := \lambda_0(1 - \eta) - R,$$

$$\bar{\lambda} := \lambda_0(1 + \eta) + R + \delta \underline{\lambda}$$

and

$$L := \frac{\bar{\lambda}}{(1 - \delta)\underline{\lambda}}.$$

Then on the set where $\hat{R} \leq R$ and $\|\varepsilon\|_n \geq \underline{\sigma}$, we have

$$\begin{aligned} & 2\delta \underline{\lambda} \|\hat{\beta} - \beta^0\|_1 \|\varepsilon\|_n + \|X(\hat{\beta} - \beta^0)\|_n^2 \\ & \leq \min_S \left\{ \min_{\beta \in \mathbb{R}^p, S_\beta = S} \left[2\delta \underline{\lambda} \|\beta - \beta^0\|_1 \|\varepsilon\|_n + \|X(\beta - \beta^0)\|_n^2 \right] + \bar{\lambda}^2 \frac{|S| \|\varepsilon\|_n^2}{\hat{\phi}^2(L, S)} \right\}. \end{aligned} \quad (12)$$

The result of Theorem 2 leads to a trade-off between the approximation error $\|X(\beta - \beta^0)\|_n^2$, the ℓ_1 -error $\|\beta - \beta^0\|_1$ and the sparseness¹ $|S_\beta|$ (or rather the *effective sparseness* $|S_\beta|/\hat{\phi}^2(L, S_\beta)$).

5 A bound for the ℓ_1 -estimation error under (weak) sparsity

In this section we assume

$$\sum_{j=1}^r |\beta_j^0|^r \leq \rho_r^r, \quad (13)$$

where $0 < r < 1$ and where $\rho_r > 0$ is a constant that is “not too large”. This is sometimes called *weak sparsity* as opposed to *strong sparsity* which requires “not too many” non-zero coefficients $s_0 := \#\{\beta_j^0 \neq 0\}$. We start with bounding the right hand side of the oracle inequality (12) in Theorem 2.

We let $S_0 := S_{\beta^0}$ be the active set $S_0 := \{j : \beta_j^0 \neq 0\}$ of β_0 and let $\hat{\Lambda}_{\max}^2(S_0)$ be the largest eigenvalue of $X_{S_0}^T X_{S_0} / n$. The cardinality of S_0 is denoted by $s_0 = |S_0|$. We assume in this section the normalization $\|X_j\|_n = 1$ so that that $\hat{\Lambda}_{\max}(S_0) \geq 1$ and $\hat{\phi}(L, S) \leq 1$ for any L and S .

¹ or non-sparseness actually

Lemma 4. Suppose β^0 satisfies the weak sparsity condition (13) for some $0 < r < 1$ and $\rho_r > 0$. For any positive $\delta, \underline{\lambda}, \bar{\lambda}$ and L

$$\begin{aligned} \min_S \left\{ \min_{\beta \in \mathbb{R}^p, S_\beta = S} \left[2\delta \underline{\lambda} \|\beta - \beta^0\|_1 \|\varepsilon\|_n + \|X(\beta - \beta^0)\|_n^2 \right] + \bar{\lambda}^2 \frac{|S| \|\varepsilon\|_n^2}{\hat{\phi}^2(L, S)} \right\} \\ \leq 2\bar{\lambda}^{2-r} \left(\delta \underline{\lambda} / \bar{\lambda} + \frac{\hat{\Lambda}_{\max}^r(S_0)}{\hat{\phi}^2(L, \hat{S}_*)} \right) \left(\frac{\rho_r}{\|\varepsilon\|_n} \right)^r \|\varepsilon\|_n^2, \end{aligned}$$

where $\hat{S}_* := \{j : |\beta_j^0| > \bar{\lambda} \|\varepsilon\|_n / \hat{\Lambda}_{\max}(S_0)\}$.

As a consequence, we obtain bounds for the prediction error and ℓ_1 -error of the square-root Lasso under (weak) sparsity. We only present the bound for the ℓ_1 -error as this is what we need in Theorem 1 for the construction of asymptotic confidence sets.

To avoid being taken away by all the constants, we make some arbitrary choices in Lemma 5: we set $\eta \leq 1/3$ in the ℓ_1 -sparsity condition (11) and we set $\lambda_0(1 - \eta) = 2R$. We choose $\delta = 1/7$.

We include the confidence statements that are given in Lemma 2 to complete the picture.

Lemma 5. Suppose $\varepsilon \sim \mathcal{N}(0, \sigma_0^2 I)$. Let α_0 and $\underline{\alpha}$ be given positive error levels such that $\alpha_0 + \underline{\alpha} < 1$ and $\log(1/\underline{\alpha}) < n/4$. Define

$$\underline{\sigma}^2 := \sigma_0^2 \left(1 - 2\sqrt{\frac{\log(1/\underline{\alpha})}{n}} \right), \quad R := \sqrt{\frac{\log(2p/\alpha_0)}{n - 2\sqrt{n\log(1/\underline{\alpha})}}}.$$

Assume the ℓ_1 -sparsity condition

$$R\|\beta^0\|_1 / \underline{\sigma} \leq (1 - \eta) \left(\sqrt{1 + (\eta/2)^2} - 1 \right), \text{ where } 0 < \eta \leq 1/3$$

and the ℓ_r -sparsity condition (13) for some $0 < r < 1$ and $\rho_r > 0$. Set

$$S_* := \{j : |\beta_j^0| > 3R\underline{\sigma} / \hat{\Lambda}_{\max}(S_0)\}.$$

Then for $\lambda_0(1 - \eta) = 2R$, with probability at least $1 - \alpha_0 - \underline{\alpha}$ we have the ℓ_r -sparsity based bound

$$(1 - \eta) \frac{\|\hat{\beta} - \beta^0\|_1}{\hat{\sigma}} \leq \frac{\|\hat{\beta} - \beta^0\|_1}{\|\varepsilon\|_n} \leq (6R)^{1-r} \left(1 + \frac{6^2 \hat{\Lambda}_{\max}^r(S_0)}{\hat{\phi}^2(6, S_*)} \right) \left(\frac{\rho_r}{\underline{\sigma}} \right)^r,$$

the ℓ_0 -sparsity based bound

$$(1 - \eta) \frac{\|\hat{\beta} - \beta^0\|_1}{\hat{\sigma}} \leq \frac{\|\hat{\beta} - \beta^0\|_1}{\|\varepsilon\|_n} \leq 3R \left(\frac{6^2 s_0}{\hat{\phi}^2(6, S_0)} \right)$$

and moreover the following lower bound for the estimator $\hat{\sigma}$ of the noise level:

$$(1 - \eta) \sigma_0 / \hat{\sigma} \leq \left(1 - 2\sqrt{\frac{\log(1/\underline{\alpha})}{n}} \right)^{-1/2}.$$

Asymptotics Application of Theorem 1 with σ_0 estimated by $\hat{\sigma}$ requires that $\sqrt{n}\lambda \|\hat{\beta} - \beta^0\|_1 / \hat{\sigma}$ tends to zero in probability. Taking $\lambda \asymp \sqrt{\log p/n}$ and for example $\alpha_0 = \alpha = 1/p$, we see that this is the case under the conditions of Lemma 5 as soon as for some $0 < r < 1$ the following ℓ_r -sparsity based bound holds:

$$\left(\frac{\hat{\Lambda}_{\max}^r(S_0)}{\hat{\phi}^2(6, S_*)}\right) \left(\frac{\rho_r}{\sigma_0}\right)^r = \frac{o(n/\log p)^{\frac{1-r}{2}}}{(\log p)^{\frac{1}{2}}}.$$

Alternatively, one may require the ℓ_0 -sparsity based bound

$$\left(\frac{1}{\hat{\phi}^2(6, S_0)}\right)^{s_0} = \frac{o(n/\log p)^{\frac{1}{2}}}{(\log p)^{\frac{1}{2}}}.$$

6 Structured sparsity

We will now show that the results hold for norm-penalized estimators with norms other than ℓ_1 . Let Ω be some norm on $\mathbb{R}^{p-|J|}$ and define for a $(p-|J|) \times |J|$ matrix $A := (a_1, \dots, a_{|J|})$

$$\|A\|_{1, \Omega} := \sum_{j=1}^{|J|} \Omega(a_j).$$

For a vector $z \in \mathbb{R}^{p-|J|}$ we define the dual norm

$$\Omega_*(z) = \sup_{\Omega(a) \leq 1} |z^T a|,$$

and for a $(p-|J|) \times |J|$ matrix $Z = (z_1, \dots, z_{|J|})$ we let

$$\|Z\|_{\infty, \Omega_*} = \max_{1 \leq j \leq |J|} \Omega_*(z_j).$$

Thus, when Ω is the ℓ_1 -norm we have $\|A\|_{1, \Omega} = \|A\|_1$ and $\|Z\|_{\infty, \Omega_*} = \|Z\|_{\infty}$. We let the multivariate square-root Ω -sparse estimator be

$$\hat{\Gamma}_J := \arg \min_{\Gamma_J} \left\{ \|X_J - X_{-J}\Gamma_J\|_{\text{nuclear}} / \sqrt{n} + \lambda \|\Gamma_J\|_{1, \Omega} \right\}.$$

This estimator equals (6) when Ω is the ℓ_1 -norm.

We let, as in (7), (8) and (10) but now with the new $\hat{\Gamma}_J$, the quantities \tilde{T}_J , \hat{T}_J and M be defined as

$$\tilde{T}_J := (X_J - X_{-J}\hat{\Gamma}_J)^T X_J / n,$$

$$\hat{T}_J := (X_J - X_{-J}\hat{\Gamma}_J)^T (X_J - X_{-J}\hat{\Gamma}_J) / n$$

and

$$M := M_{\lambda} := \sqrt{n} \hat{T}_J^{-1/2} \tilde{T}_J.$$

The Ω -de-sparsified estimator of β_J^0 is as in Definition 1

$$\hat{b}_J := \hat{\beta}_J + \tilde{T}_J^{-1} (X_J - X_{-J}\hat{\Gamma}_J)^T (Y - X\hat{\beta}) / n,$$

but now with $\hat{\beta}$ not necessarily the square root Lasso but a suitably chosen initial estimator and with $\hat{\Gamma}_J$ the multivariate square-root Ω -sparse estimator. The normalized de-sparsified estimator is $M\hat{b}_J$ with normalization matrix M given above. We can then easily derive the following extension of Theorem 1.

Theorem 3. Consider the model $Y \sim \mathcal{N}_n(f^0, \sigma_0^2)$ where $f^0 = X\beta^0$. Let \hat{b}_J be the Ω -de-sparsified estimator depending on some initial estimator $\hat{\beta}$. Let $M\hat{b}_J$ be its normalized version. Then

$$M(\hat{b}_J - \beta_J^0)/\sigma_0 = \mathcal{N}_{|J|}(0, I) + \text{rem}$$

where $\|\text{rem}\|_\infty \leq \sqrt{n}\lambda\Omega(\hat{\beta}_{-J} - \beta_{-J}^0)/\sigma_0$.

We see from Theorem 3 that confidence sets follow from fast rates of convergence of the Ω -estimation error. The latter is studied in Bach [2010], Obozinski and Bach [2012] and van de Geer [2014] for the case where the initial estimator is the least squares estimator with penalty based on a sparsity inducing norm $\bar{\Omega}$ (say). Group sparsity Yuan and Lin [2006] is an example which we shall now briefly discuss.

Example 1. Let G_1, \dots, G_T be given mutually disjoint subsets of $\{1, \dots, p\}$ and take as sparsity-inducing norm

$$\bar{\Omega}(\beta) := \sum_{t=1}^T \sqrt{|G_t|} \|X\beta_{G_t}\|_2, \beta \in \mathbb{R}^p.$$

The group Lasso is the minimizer of least squares loss with penalty proportional to $\bar{\Omega}$. Oracle inequalities for the $\bar{\Omega}$ -error of the group Lasso have been derived in Lounici et al. [2011] for example. For the square-root version we refer to Bunea et al. [2013]. With group sparsity, it lies at hand to consider confidence sets for one of the groups G_t i.e., to take $J = G_{t_0}$ for a given t_0 . Choosing

$$\Omega(a) = \sum_{t \neq t_0} \sqrt{|G_t|} \|Xa_{G_t}\|_2, a \in \mathbb{R}^{p-|G_{t_0}|}$$

will ensure that $\Omega(\hat{\beta}_{-G_{t_0}} - \beta_{-G_{t_0}}) \leq \bar{\Omega}(\hat{\beta} - \beta^0)$ which gives one a handle to control the remainder term in Theorem 3. This choice of Ω for constructing the confidence set makes sense if one believes that the group structure describing the relation between the response Y and the input X is also present in the relation between $X_{G_{t_0}}$ and $X_{-G_{t_0}}$.

7 Simulations

Here we denote by $\tilde{Y} = \tilde{X}B_0 + \varepsilon$ an arbitrary linear multivariate regression. In a similar fashion to the square-root Algorithm in Buena et al. (2014) we propose the following algorithm for the multivariate square-root Lasso:

Algorithm 1 msrL

Require: Take a constant K big enough, and choose an arbitrary starting matrix $B(0) \in \mathbb{R}^{p \times q}$.

- 1: $\tilde{Y} \leftarrow \tilde{Y}/K$
 - 2: $\tilde{X} \leftarrow \tilde{X}/K$
 - 3: **for** $t = 0, 1, 2, \dots, t_{\text{stop}}$ **do**
 - 4: $B(t+1) := \bar{\Phi}(B(t) + X^T \cdot (Y - XB(t)); \lambda \|Y - XB(t)\|_{\text{nuclear}})$
 - 5: **return** $B(t_{\text{stop}} + 1)$
-

Here we denote

$$\bar{\Phi}(a; \eta) := \begin{cases} 0, & \text{if } a = 0 \\ \frac{a}{\|a\|_2} (\|a\|_2 - \eta)_+, & \text{if } a > 0 \end{cases}.$$

The value t_{stop} can be chosen in such a way that one gets the desired accuracy for the algorithm. This algorithm is based on a Fixpoint equation from the KKT conditions. The square root Lasso is calculated via the algorithm in Buena et al. (2014).

We consider the usual linear regression model:

$$Y = X\beta + \varepsilon.$$

In our simulations we take a design matrix X , where the rows are fixed i.i.d. realizations from $\mathcal{N}(0, \Sigma)$. We have n observations, and p explanatory variables. The covariance matrix Σ has the following toeplitz structure $\Sigma_{i,j} = 0.9^{|i-j|}$. The errors are i.i.d. Gaussian distributed, with variance $\sigma^2 = 1$. A set of points J is also chosen. J denotes the set of indices of the parameter vector β that we want to find asymptotic group confidence intervals for. Define as $q = |J|$ the number of indices of interest. For each different setting of p and n we do $r = 1000$ simulations. In each repetition we calculate the teststatistic χ^2 . A significance level of 0.05 is chosen. The lambda of the square root LASSO λ_{srL} in the simulations is the theoretical lambda λ_{srLt} scaled by 3. For the lambda of the multivariate square root LASSO λ_{msrL} we do not have theoretical results yet. That is why we use cross-validation where we minimize the error expressed in nuclear norm, to define λ_{msrL} . It is important to note, that the choice of λ_{msrL} is very crucial, especially for cases where n is small. One could tune λ_{msrL} in such a fashion that even cases like $n = 100$ work much better, see figure 2. But the point here is to see what happens to the chi-squared test statistic with a fixed rule for the choice of λ_{msrL} . This basic set up is used throughout all the simulations below.

7.1 Asymptotic distribution

First let us look at the question how the histogram of the teststatistic looks like for different n . Here we use $p = 500$ and $q = 6$ with $J = (1, 3, 4, 8, 10, 33)$, where the entries in β_J are chosen randomly from a Uniform distribution on $[1, 4]$. We also specify β_{-J} to be the zero vector. So the set J that we are interested in, is in fact the same set as the active set of β . Furthermore $p - q$ gives the amount of sparsity. Here we look at a sequence of $n = 100, 200, 300, 400, 500, 600, 800$. As above, for each setting we calculate 1000 simulations. For each setting we plot the histogram for the teststatistic and compare it with the theoretical chi-squared distribution on $q = 6$ degrees of freedom. Figure 1 and figure 2 show the results.

The histograms show that with increasing n , we get a fast convergence to the true asymptotic chi-squared distribution. It is in fact true that we could multiply the teststatistic with a constant $C_n \leq 1$ in order to get the histogram match the chi-squared distribution. This reflects the theory. Already with $n = 400$ we get a very good approximation of the chi-squared distribution. But we see that the tuning of λ_{msrL} is crucial for small n , see figure 2.

Next we try the same procedure but we are interested in what happens if we let J and the active set S_0 not be the same set. Here we take $J = (1, 3, 4, 8, 10, 33)$ and β_0 is taken from the uniform distribution on $[1, 4]$ on the set $S_0 = (2, 3, 5, 8, 11, 12, 14, 31)$. So only the indices $J \cap S_0 = \{3, 8\}$ coincide. Figure 3 shows the results.

Compared to the case where J and S_0 are the same set, it seems that this setting can handle small n better than in the case where all the elements of J are the nonzero indices of β_0 . So the previous case seems to be the harder case. Therefore we stick with $J = S_0 = (1, 3, 4, 8, 10, 33)$ for all the other simulations in Subsection 7.2 and 7.3.

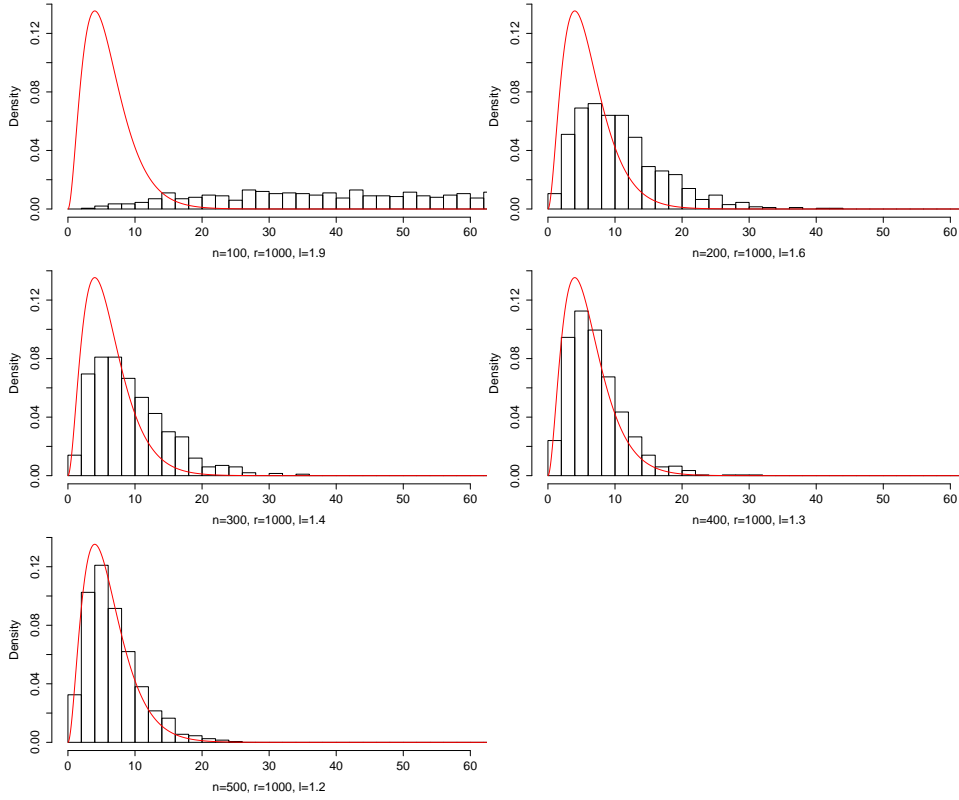


Fig. 1 Histogram of Teststatistic, $l=\lambda$, the cross-validation lambda

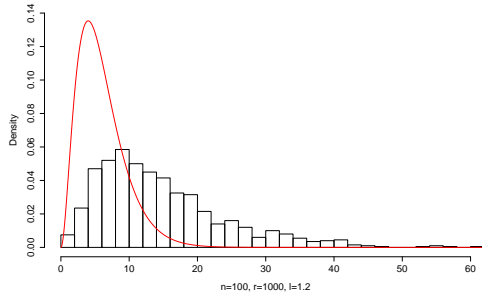


Fig. 2 Histogram of Teststatistic with a tuned $\lambda_{msrL}=l=1.2$ for $n = 100$

7.2 Confidence level for an increasing λ_{msrL}

Up until now we have not looked at the behaviour for different λ . We only used the cross-validation λ . So here we look at $n = 400$, $p = 500$ and we take $\lambda_{msrL} = (0.01, 0.11, 0.21, \dots, 2.91)$ a fixed sequence. Figure 4 shows the results.

If we take λ too low the behaviour breaks down. On the other hand, if λ is too big, we will not achieve a good average confidence level. The cross-validation λ seems to be still a bit too high. So the cross-validation λ could be better.

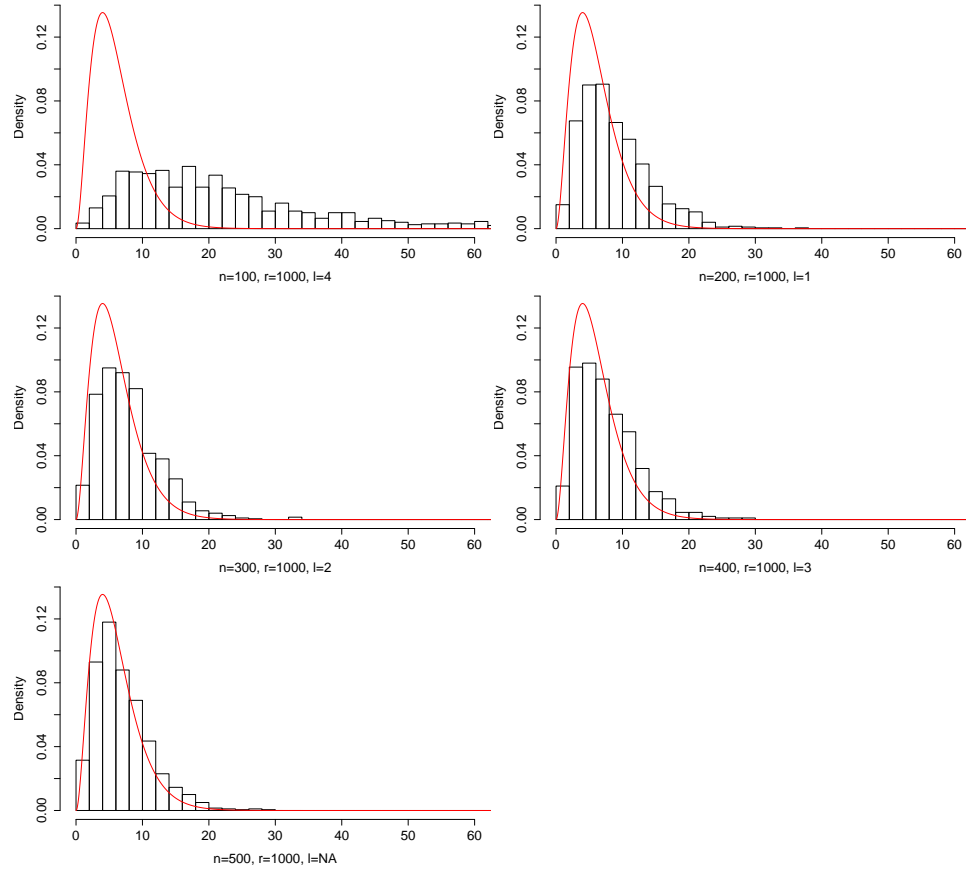


Fig. 3 Histogram of Teststatistic, $l=\lambda$, the cross-validation lambda

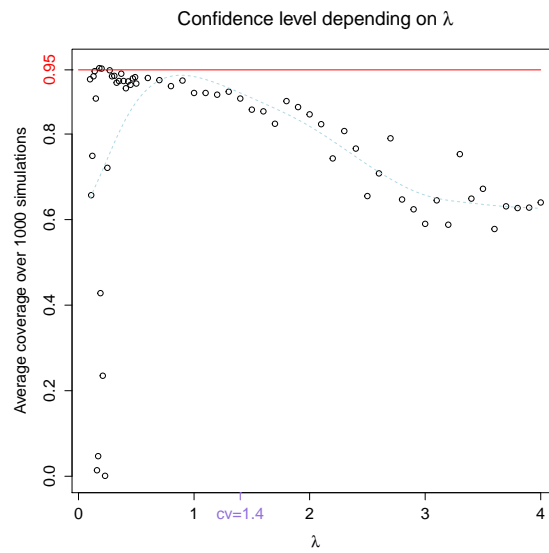


Fig. 4 Average confidence level with fixed $n = 400$ and $p = 500$, increased λ

7.3 Levelplot for n and p

Not let us look at an overview of alot of different settings. We will use the levelplot to present the results Here we use the cross-validation λ . We let n and p increase and look again at the average coverage of the confidence interval (average over the 1000 simulations for each gridpoint). The border between high and low dimensional cases is marked by the white line in figure 5. Increasing p does not worsen the procedure too much, which is very good. And, as expected, increasing the number of observations n increases "the accuracy" of the average confidence interval.

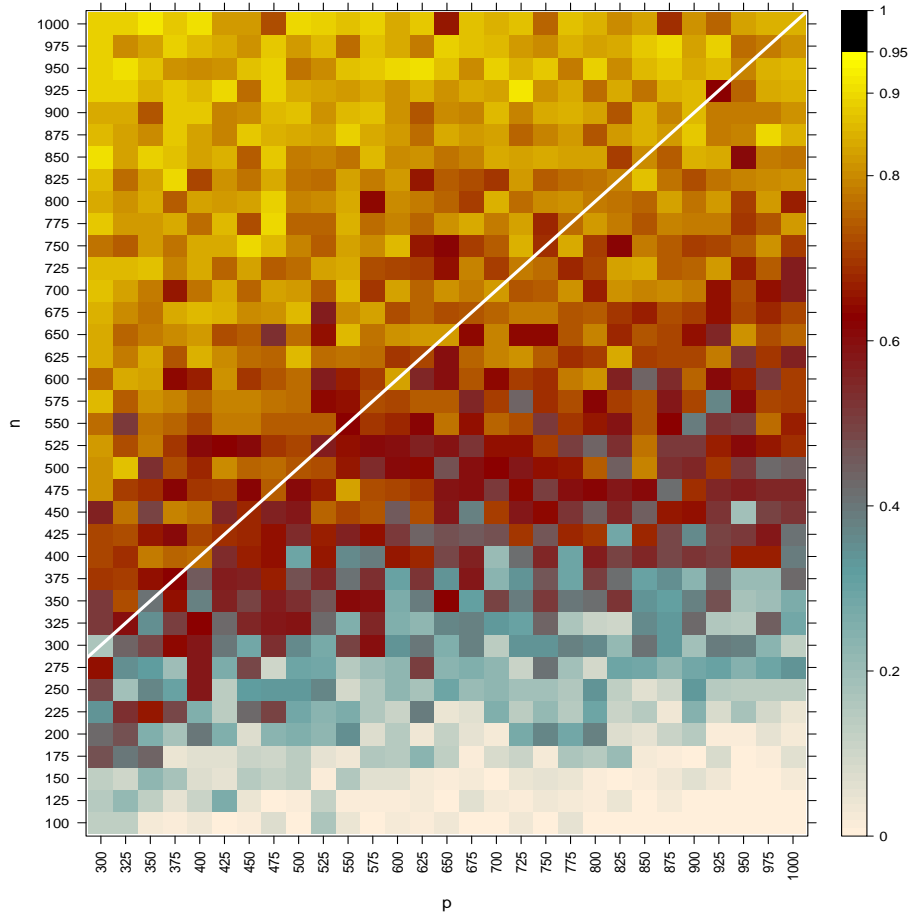


Fig. 5 Levelplot of average confidence level for a grid n, p

8 Discussion

We have presented a method for constructing confidence sets for groups of variables which does not impose sparsity conditions on the input matrix X . The idea is to use a loss function based on the nuclear norm of the matrix of residuals. We called this the multivariate square-root Lasso as it is an extension of the square-root Lasso in the multivariate case.

It is easy to see that when the groups are large, one needs the ℓ_2 -norm of the remainder term $\|\text{rem}\|^2$ in Theorem 1 to be of small order $\sqrt{|J|}$ in probability, using the representation $\chi_{|J|}^2 = |J| + O_P(\sqrt{|J|})$. This leads to the requirement that $\sqrt{n}\lambda\|\hat{\beta}_{-J} - \beta_j^0\|_1/\sigma_0 = o_P(1/|J|^{1/4})$, i.e., that it decreases faster for large groups. The paper Mitra and Zhang [2014] introduces a different scheme for confidence sets, where there is no dependence on group size in the remainder term after the normalization for large groups. Their idea is to use a group Lasso with a nuclear norm type of penalty on Γ_J instead of the ℓ_1 -norm $\|\Gamma_J\|_1$ as we do in Theorem 1. Combining the approach of Mitra and Zhang [2014] with the result of Theorem 3 leads to a new remainder term which after normalization for large groups does not depend on group size *and* does not rely on sparsity assumptions on the design X .

The choice of the tuning parameter λ for the construction used in Theorem 1 is as yet an open problem. When one is willing to assume certain sparsity assumptions such that a bound for $\|\hat{\beta} - \beta^0\|_1$ is available, the tuning parameter can be chosen by trading off the size of the confidence set and the bias. When the rows of X are i.i.d. random variables, a choice for λ of order $\sqrt{\log p/n}$ is theoretically justified under certain conditions. Finally, smaller λ give more conservative confidence intervals. Thus, increasing λ will give one a “solution path” of significant variables entering and exiting, where the number of “significant” variables increases. If one aims at finding potentially important variables, one might want to choose a cut-off level here, i.e. choose λ in such a way that the number of “significant” variables is equal to a prescribed number. However, we have as yet no theory showing such a data-dependent choice of λ is meaningful.

A given value for λ may yield sets which do not have the approximate coverage. These sets can nevertheless be viewed as giving a useful importance measure for the variables, an importance measure which avoids the possible problems of other methods for accessing accuracy. For example, when applied to all variables (after grouping) the confidence sets clearly also give results for the possibly weak variables. This is in contrast to post-model selection where the variables not selected are no longer under consideration.

9 Proofs

9.1 Proof for the result for the multivariate square-root Lasso in Subsection 2.2

Proof of Lemma 1. Let us write, for each $p \times q$ matrix B , the residuals as $\Sigma(B) := (Y - XB)^T(Y - XB)/n$. Let $\Sigma_{\min}(B)$ be the minimizer of

$$\text{trace}(\Sigma(B)\Sigma^{-1/2}) + \text{trace}(\Sigma^{1/2}) \quad (14)$$

over Σ . Then $\Sigma_{\min}(B)$ equals $\Sigma(B)$. To see this we invoke the reparametrization $\Omega := \Sigma^{-1/2}$ so that $\Sigma^{1/2} = \Omega^{-1}$. We now minimize

$$\text{trace}(\Sigma(B)\Omega) + \text{trace}(\Omega^{-1})$$

over $\Omega > 0$. The matrix derivative with respect to Ω of $\text{trace}(\Sigma(B)\Omega)$ is $\Sigma(B)$. The matrix derivative of $\text{trace}(\Omega^{-1})$ with respect to Ω is equal to $-\Omega^{-2}$. Hence the minimizer $\Omega_{\min}(B)$ satisfies the equation

$$\Sigma(B) - \Omega_{\min}^{-2}(B) = 0,$$

giving

$$\Omega_{\min}(B) = \Sigma^{-1/2}(B).$$

so that

$$\Sigma_{\min}(B) = \Omega_{\min}^{-2}(B) = \Sigma(B).$$

Inserting this solution back in (14) gives $2\text{trace}(\Sigma^{1/2}(B))$ which is equal to $2\|Y - XB\|_{\text{nuclear}}/\sqrt{n}$. This proves the first part of the lemma.

Let now for each $\Sigma > 0$, $B(\Sigma)$ be the minimizer of

$$\text{trace}(\Sigma(B)\Sigma^{-1/2}) + 2\lambda_0\|B\|_1.$$

By sub-differential calculus we have

$$X^T(Y - XB)\Sigma^{-1/2}/n = \lambda_0 Z(\Sigma)$$

where $\|Z(\Sigma)\|_{\infty} \leq 1$ and $Z_{k,j}(\Sigma) = \text{sign}(B_{k,j}(\Sigma))$ if $B_{k,j}(\Sigma) \neq 0$ ($k = 1, \dots, p$, $j = 1, \dots, q$). The KKT-conditions (5) follow from $\hat{B} = B(\hat{\Sigma})$. \square

9.2 Proof of the main result in Subsection 3.2

Proof of Theorem 1. We have

$$\begin{aligned} M(\hat{b}_J - \hat{\beta}_J) &= \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T \varepsilon / \sqrt{n} - \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T X(\hat{\beta} - \beta^0) / \sqrt{n} \\ &= \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T \varepsilon / \sqrt{n} - \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T X_J(\hat{\beta}_J - \beta_J^0) / \sqrt{n} \\ &\quad - \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T X_{-J}(\hat{\beta}_{-J} - \beta_{-J}^0) / \sqrt{n} \\ &= \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T \varepsilon / \sqrt{n} - M(\hat{\beta}_J - \beta_J^0) - \sqrt{n}\lambda \hat{Z}_J^T(\hat{\beta}_{-J} - \beta_{-J}^0) \end{aligned}$$

where we invoked the KKT-conditions (9). We thus arrive at

$$M(\hat{b}_J - \beta_J^0) = \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T \varepsilon / \sqrt{n} + \sigma_0 \text{rem}, \quad (15)$$

where

$$\text{rem} = -\sqrt{n}\lambda \hat{Z}_J^T(\hat{\beta}_{-J} - \beta_{-J}^0) / \sigma_0.$$

The co-variance matrix of the first term $\hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T \varepsilon / \sqrt{n}$ in (15) is equal to

$$\sigma_0^2 \hat{T}_J^{-1/2}(X_J - X_{-J}\hat{T}_J)^T (X_J - X_{-J}\hat{T}_J) \hat{T}_J^{-1/2} / n = \sigma_0^2 I$$

where I is the identity matrix with dimensions $|J| \times |J|$. It follows that this term is $|J|$ -dimensional standard normal scaled with σ_0 . The remainder term can be bounded using the dual norm inequality for each entry:

$$|\text{rem}_j| \leq \sqrt{n}\lambda \max_{k \notin J} |(\hat{Z}_J)_{k,j}| \|\hat{\beta}_{-J} - \beta_{-J}^0\|_1 / \sigma_0 \leq \sqrt{n}\lambda \|\hat{\beta}_{-J} - \beta_{-J}^0\|_1 / \sigma_0$$

since by the KKT-conditions (9), we have $\|\hat{Z}_J\|_{\infty} \leq 1$. \square

9.3 Proofs of the theoretical result for the square-root Lasso in Section 4

Proof of Lemma 2. Without loss of generality we can assume $\sigma_0^2 = 1$. From Laurent and Massart [2000] we know that for all $t > 0$

$$\mathbf{P}\left(\|\varepsilon\|_n^2 \leq 1 - 2\sqrt{t/n}\right) \leq \exp[-t]$$

and

$$\mathbf{P}\left(\|\varepsilon\|_n^2 \geq 1 + 2\sqrt{t/n} + 2t/n\right) \leq \exp[-t].$$

Apply this with $t = \log(1/\underline{\alpha})$ and $t = \log(1/\bar{\alpha})$ respectively. Moreover $X_j^T \varepsilon/n \sim \mathcal{N}(0, 1/n)$ for all j . Hence for all $t > 0$

$$\mathbf{P}\left(|X_j^T \varepsilon|/n \geq \sqrt{2t/n}\right) \leq 2\exp[-t], \forall j.$$

It follows that

$$\mathbf{P}\left(\|X^T \varepsilon\|_\infty/n \geq \sqrt{2(t + \log(2p))/n}\right) \leq \exp[-t].$$

□

Proof of Lemma 3. Suppose $\hat{R} \leq R$ and $\|\varepsilon\|_n \geq \underline{\sigma}$. First we note that the inequality (11) gives

$$\lambda_0 \|\beta^0\|_1 / \|\varepsilon\|_n \leq 2 \left(\sqrt{1 + (\eta/2)^2} - 1 \right).$$

For the upper bound for $\|\hat{\varepsilon}\|_n$ we use that

$$\|\hat{\varepsilon}\|_n + \lambda_0 \|\hat{\beta}\|_1 \leq \|\varepsilon\|_n + \lambda_0 \|\beta^0\|_1$$

by the definition of the estimator. Hence

$$\|\hat{\varepsilon}\|_n \leq \|\varepsilon\|_n + \lambda_0 \|\beta^0\|_1 \leq \left[1 + 2 \left(\sqrt{1 + (\eta/2)^2} - 1 \right) \right] \|\varepsilon\|_n \leq (1 + \eta) \|\varepsilon\|_n.$$

For the lower bound for $\|\hat{\varepsilon}\|_n$ we use the convexity of both the loss function and the penalty. Define

$$\alpha := \frac{\eta \|\varepsilon\|_n}{\eta \|\varepsilon\|_n + \|X(\hat{\beta} - \beta^0)\|_n}.$$

Note that $0 < \alpha \leq 1$. Let $\hat{\beta}_\alpha$ be the convex combination $\hat{\beta}_\alpha := \alpha \hat{\beta} + (1 - \alpha) \beta^0$. Then

$$\|X(\hat{\beta}_\alpha - \beta^0)\|_n = \alpha \|X(\hat{\beta} - \beta^0)\|_n = \frac{\eta \|\varepsilon\|_n \|X(\hat{\beta} - \beta^0)\|_n}{\eta \|\varepsilon\|_n + \|X(\hat{\beta} - \beta^0)\|_n} \leq \eta \|\varepsilon\|_n.$$

Define $\hat{\varepsilon}_\alpha := Y - X\hat{\beta}_\alpha$. Then, by convexity of $\|\cdot\|_n$ and $\|\cdot\|_1$,

$$\begin{aligned} \|\hat{\varepsilon}_\alpha\|_n + \lambda_0 \|\hat{\beta}_\alpha\|_1 &\leq \alpha \|\hat{\varepsilon}\|_n + \alpha \lambda_0 \|\hat{\beta}\|_1 + (1 - \alpha) \|\varepsilon\|_n + (1 - \alpha) \lambda_0 \|\beta^0\|_1 \\ &\leq \|\varepsilon\|_n + \lambda_0 \|\beta^0\|_1 \end{aligned}$$

where in the last step we again used that $\hat{\beta}$ minimizes $\|Y - X\beta\|_n + \lambda_0 \|\beta\|_1$. Taking squares on both sides gives

$$\|\hat{\epsilon}_\alpha\|_n^2 + 2\lambda_0\|\hat{\beta}_\alpha\|_1\|\epsilon\|_n + \lambda_0^2\|\hat{\beta}_\alpha\|_1^2 \leq \|\epsilon\|_n^2 + 2\lambda_0\|\beta^0\|_1\|\epsilon\|_n + \lambda_0^2\|\beta^0\|_1^2. \quad (16)$$

But

$$\begin{aligned} \|\hat{\epsilon}_\alpha\|_n^2 &= \|\epsilon\|_n^2 - 2\epsilon^T X(\hat{\beta}_\alpha - \beta^0)/n + \|X(\hat{\beta}_\alpha - \beta^0)\|_n^2 \\ &\geq \|\epsilon\|_n^2 - 2R\|\hat{\beta}_\alpha - \beta^0\|_1\|\epsilon\|_n + \|X(\hat{\beta}_\alpha - \beta^0)\|_n^2 \\ &\geq \|\epsilon\|_n^2 - 2R\|\hat{\beta}_\alpha\|_1\|\epsilon\|_n - 2R\|\beta^0\|_1\|\epsilon\|_n + \|X(\hat{\beta}_\alpha - \beta^0)\|_n^2. \end{aligned}$$

Moreover, by the triangle inequality

$$\|\hat{\epsilon}_\alpha\|_n \geq \|\epsilon\|_n - \|X(\hat{\beta}_\alpha - \beta^0)\|_n \geq (1 - \eta)\|\epsilon\|_n.$$

Inserting these two inequalities into (16) gives

$$\begin{aligned} \|\epsilon\|_n^2 - 2R\|\hat{\beta}_\alpha\|_1\|\epsilon\|_n - 2R\|\beta^0\|_1\|\epsilon\|_n + \|X(\hat{\beta}_\alpha - \beta^0)\|_n^2 + 2\lambda_0(1 - \eta)\|\hat{\beta}_\alpha\|_1\|\epsilon\|_n + \lambda_0^2\|\hat{\beta}_\alpha\|_1^2 \\ \leq \|\epsilon\|_n^2 + 2\lambda_0\|\beta^0\|_1\|\epsilon\|_n + \lambda_0^2\|\beta^0\|_1^2 \end{aligned}$$

which implies by the assumption $\lambda_0(1 - \eta) \geq R$

$$\begin{aligned} \|X(\hat{\beta}_\alpha - \beta^0)\|_n^2 &\leq 2(\lambda_0 + R)\|\beta^0\|_1\|\epsilon\|_n + \lambda_0^2\|\beta^0\|_1^2 \\ &\leq 4\lambda_0\|\beta^0\|_1\|\epsilon\|_n + \lambda_0^2\|\beta^0\|_1^2 \end{aligned}$$

where in the last inequality we used $R \leq (1 - \eta)\lambda_0 \leq \lambda_0$. But continuing we see that we can write the last expression as

$$4\lambda_0\|\beta^0\|_1\|\epsilon\|_n + \lambda_0^2\|\beta^0\|_1^2 = \left((\lambda_0\|\beta^0\|_1/\|\epsilon\|_n + 2)^2 - 4 \right) \|\epsilon\|_n^2.$$

Again invoke the ℓ_1 -sparsity condition

$$\lambda_0\|\beta^0\|_1/\|\epsilon\|_n \leq 2\left(\sqrt{1 + (\eta/2)^2} - 1\right)$$

to get

$$\left((\lambda_0\|\beta^0\|_1/\|\epsilon\|_n + 2)^2 - 4 \right) \|\epsilon\|_n^2 \leq \frac{\eta^2}{4} \|\epsilon\|_n^2.$$

We thus established that

$$\|X(\hat{\beta}_\alpha - \beta^0)\|_n \leq \frac{\eta\|\epsilon\|_n}{2}.$$

Rewrite this to

$$\frac{\eta\|\epsilon\|_n\|X(\hat{\beta}_\alpha - \beta^0)\|_n}{\eta\|\epsilon\|_n + \|X(\hat{\beta}_\alpha - \beta^0)\|_n} \leq \frac{\eta\|\epsilon\|_n}{2},$$

and rewrite this in turn to

$$\eta\|\epsilon\|_n\|X(\hat{\beta}_\alpha - \beta^0)\|_n \leq \frac{\eta^2\|\epsilon\|_n^2}{2} + \frac{\eta\|\epsilon\|_n\|X(\hat{\beta}_\alpha - \beta^0)\|_n}{2}$$

or

$$\|X(\hat{\beta}_\alpha - \beta^0)\|_n \leq \eta\|\epsilon\|_n.$$

But then, by repeating the argument, also

$$\|\hat{\epsilon}\|_n \geq \|\epsilon\|_n - \|X(\hat{\beta}_\alpha - \beta^0)\|_n \geq (1 - \eta)\|\epsilon\|_n.$$

□

Proof of Theorem 2. Throughout the proof we suppose $\hat{R} \leq R$ and $\|\varepsilon\|_n \geq \underline{\sigma}$. Define the Gram matrix $\hat{\Sigma} := X^T X/n$. Let $\beta \in \mathbb{R}^p$ and $S := S_\beta = \{j : \beta_j \neq 0\}$. If

$$(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) \leq -\delta \underline{\lambda} \|\hat{\beta} - \beta\|_1 \|\varepsilon\|_n$$

we find

$$\begin{aligned} & 2\delta \underline{\lambda} \|\hat{\beta} - \beta\|_1 \|\varepsilon\|_n + \|X(\hat{\beta} - \beta^0)\|_n^2 \\ &= 2\delta \underline{\lambda} \|\hat{\beta} - \beta\|_1 \|\varepsilon\|_n + \|X(\beta - \beta^0)\|_n^2 - \|X(\beta - \hat{\beta})\|_n^2 + 2(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) \\ &\leq \|X(\beta - \beta^0)\|_n^2. \end{aligned}$$

So then we are done.

Suppose now that

$$(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) \geq -\delta \underline{\lambda} \|\hat{\beta} - \beta\|_1 \|\varepsilon\|_n.$$

By the KKT-conditions (3)

$$(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) + \lambda_0 \|\hat{\beta}\|_1 \|\hat{\varepsilon}\|_n \leq \varepsilon^T X(\hat{\beta} - \beta)/n + \lambda_0 \|\beta\|_1 \|\hat{\varepsilon}\|_n.$$

By the dual norm inequality and since $\hat{R} \leq R$

$$|\varepsilon^T X(\hat{\beta} - \beta)|/n \leq R \|\hat{\beta} - \beta\|_1 \|\varepsilon\|_n.$$

Thus

$$(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) + \lambda_0 \|\hat{\beta}\|_1 \|\hat{\varepsilon}\|_n \leq R \|\hat{\beta} - \beta\|_1 \|\varepsilon\|_n + \lambda_0 \|\beta\|_1 \|\hat{\varepsilon}\|_n.$$

This implies by the triangle inequality

$$(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) + (\lambda_0 \|\hat{\varepsilon}\|_n - R \|\varepsilon\|_n) \|\hat{\beta}_{-S}\|_1 \leq (\lambda_0 \|\hat{\varepsilon}\|_n + R \|\varepsilon\|_n) \|\hat{\beta}_S - \beta\|_1.$$

We invoke the result of Lemma 3 which says that that $(1 - \eta) \|\varepsilon\|_n \leq \|\hat{\varepsilon}\|_n \leq (1 + \eta) \|\varepsilon\|_n$.

This gives

$$(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) + \underline{\lambda} \|\hat{\beta}_{-S}\|_1 \|\varepsilon\|_n \leq (\lambda_0(1 + \eta) + R) \|\hat{\beta}_S - \beta\|_1 \|\varepsilon\|_n. \quad (17)$$

Since $(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) \geq -\delta \underline{\lambda} \|\varepsilon\|_n \|\hat{\beta} - \beta\|_1$ this gives

$$(1 - \delta) \underline{\lambda} \|\hat{\beta}_{-S}\|_1 \|\varepsilon\|_n \leq (\lambda_0(1 + \eta) + R + \delta \underline{\lambda}) \|\hat{\beta}_S - \beta\|_1 \|\varepsilon\|_n = \bar{\lambda} \|\hat{\beta}_S - \beta\|_1 \|\varepsilon\|_n.$$

or

$$\|\hat{\beta}_{-S}\|_1 \leq L \|\hat{\beta}_S - \beta\|_1.$$

But then

$$\|\hat{\beta}_S - \beta\|_1 \leq \sqrt{|S|} \|X(\hat{\beta} - \beta)\|_n / \hat{\phi}(L, S). \quad (18)$$

Continue with inequality (17) and apply the inequality $ab \leq (a^2 + b^2)/2$ which holds for all real valued a and b :

$$\begin{aligned} & (\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) + \underline{\lambda} \|\hat{\beta}_{-S}\|_1 \|\varepsilon\|_n + \delta \underline{\lambda} \|\hat{\beta}_S - \beta\|_1 \|\varepsilon\|_n \\ &\leq \bar{\lambda} \|\varepsilon\|_n \sqrt{|S|} \|X(\hat{\beta} - \beta)\|_n / \hat{\phi}(L, S) \\ &\leq \frac{1}{2} \bar{\lambda}^2 \frac{|S| \|\varepsilon\|_n^2}{\hat{\phi}^2(L, S)} + \frac{1}{2} \|X(\hat{\beta} - \beta)\|_n^2. \end{aligned}$$

Since

$$2(\hat{\beta} - \beta)^T \hat{\Sigma} (\hat{\beta} - \beta^0) = \|X(\hat{\beta} - \beta^0)\|_n^2 - \|X(\beta - \beta^0)\|_n^2 + \|X(\hat{\beta} - \beta)\|_n^2,$$

we obtain

$$\begin{aligned} & \|X(\hat{\beta} - \beta^0)\|_n^2 + 2\bar{\lambda}\|\hat{\beta}_{-S}\|_1\|\varepsilon\|_n + 2\delta\bar{\lambda}\|\hat{\beta}_S - \beta\|_1\|\varepsilon\|_n \\ & \leq \|X(\beta - \beta^0)\|_n^2 + \bar{\lambda}^2|S|\|\varepsilon\|_n^2/\hat{\phi}^2(L, S). \end{aligned}$$

□

9.4 Proofs of the illustration assuming (weak) sparsity in Section 5

Proof of Lemma 4. Define $\lambda_* := \bar{\lambda}\|\varepsilon\|_n/\hat{\Lambda}_{\max}(S_0)$ and for $j = 1, \dots, p$,

$$\beta_j^* = \beta_j^0 \mathbf{1}_{\{|\beta_j^0| > \lambda_*\}}.$$

Then

$$\begin{aligned} & \|X(\beta^* - \beta^0)\|_n^2 \leq \hat{\Lambda}_{\max}^2(S_0)\|\beta^* - \beta^0\|_2^2 \leq \hat{\Lambda}_{\max}^2(S_0)\lambda_*^{2-r}\rho_r^r \\ & = \bar{\lambda}^{2-r}\hat{\Lambda}_{\max}^r(S_0)\rho_r^r\|\varepsilon\|_n^{2-r} \leq \bar{\lambda}^{2-r}\hat{\Lambda}_{\max}^r(S_0)\rho_r^r\|\varepsilon\|_n^{2-r}/\hat{\phi}^2(L, S_*) \end{aligned}$$

where in the last inequality we used $\hat{\phi}(L, S_*) \leq 1$. Moreover, noting that $S_{\beta^*} = \hat{S}_* = \{j : |\beta_j^0| > \lambda_*\}$ we get

$$|S_{\beta^*}| \leq \lambda_*^{-r}\rho_r^r = \bar{\lambda}^{-r}\|\varepsilon\|_n^{-r}\hat{\Lambda}_{\max}^r(S_0).$$

Thus

$$\bar{\lambda}^2|S_{\beta^*}|\|\varepsilon\|_n^2/\hat{\phi}^2(L, S_{\beta^*}) \leq \bar{\lambda}^{2-r}\hat{\Lambda}_{\max}^r(S_0)\rho_r^r\|\varepsilon\|_n^{2-r}/\hat{\phi}^2(L, \hat{S}_*).$$

Moreover

$$\|\beta^* - \beta_0\|_1 \leq \lambda_*^{1-r}\rho_r^r = \bar{\lambda}^{1-r}\|\varepsilon\|_n^{1-r}\hat{\Lambda}_{\max}^r(S_0)/\hat{\phi}^2(L, \hat{S}_*),$$

since $\hat{\phi}^2(L, \hat{S}_*)/\hat{\Lambda}_{\max}(S_0) \leq 1$. □

Proof of Lemma 5. The ℓ_1 -sparsity condition (11) holds with $\eta \leq 1/3$. Theorem 2 with $\lambda_0(1 - \eta) = 2R$ gives $\underline{\lambda} = \lambda_0(1 - \eta) - R = R$ and $3R \leq \bar{\lambda} = \lambda_0(1 + \eta) + R + \delta\bar{\lambda} \leq (5 + \delta)R$. We take $\delta = 1/7$. Then $L = \bar{\lambda}/((1 - \delta)\underline{\lambda}) \leq (5 + \delta)/(1 - \delta) = 6$. Set $\hat{S}_* := \{j : |\beta_j^0| > \bar{\lambda}\|\varepsilon\|_n/\hat{\Lambda}_{\max}(S_0)\}$. On the set where $\|\varepsilon\|_n \geq \underline{\sigma}$ we have $\hat{S}_* \subset S_*$ since $\bar{\lambda} \geq 3R$. We also have $\bar{\lambda}/(\delta\underline{\lambda}) \leq 6^2$. Hence, using the arguments of Lemma 4 and the result of Theorem 2, we get on the set $\hat{R} \leq R$ and $\|\varepsilon\|_n \geq \underline{\sigma}$,

$$\frac{\|\hat{\beta} - \beta^0\|_1}{\|\varepsilon\|_n} \leq \bar{\lambda}^{1-r} \left(1 + \frac{6^2\hat{\Lambda}_{\max}^r(S_0)}{\hat{\phi}^2(6, S_*)}\right) \left(\frac{\rho_r}{\|\varepsilon\|_n}\right)^r.$$

Again, we can bound here $1/\|\varepsilon\|_n$ by $1/\underline{\sigma}$. We can moreover bound $\bar{\lambda}$ by $6R$. Next we see that on the set where $\hat{R} \leq R$ and $\|\varepsilon\|_n \geq \underline{\sigma}$, by Lemma 3,

$$\hat{\sigma} \geq (1 - \eta)\|\varepsilon\|_n \geq (1 - \eta)\underline{\sigma}.$$

The ℓ_0 -bound follows in the same way, inserting $\beta = \beta^0$ in Theorem 1. Invoke Lemma 2 to show that the set $\{\hat{R} \leq R \cap \|\varepsilon\|_n \geq \underline{\sigma}\}$ has probability at least $1 - \alpha_0 - \underline{\alpha}$. □

9.5 Proof of the extension to structured sparsity in Section 6

Proof of Theorem 3. This follows from exactly the same arguments as used in the proof of Theorem 1 as the KKT-conditions (9) with general norm Ω imply that

$$\|X_{-J}^T(X_J - X_{-J}\hat{\Gamma}_J)\hat{\Gamma}_J^{-1/2}/n\|_{\infty, \Omega_*} \leq \lambda.$$

□

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